

and other penalties.

FILE 'HOME' ENTERED AT 10:10:21 ON 24 JUN 2009

=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE  
ENTRY  
SESSION  
TOTAL  
0.22  
0.22

FILE 'REGISTRY' ENTERED AT 10:10:40 ON 24 JUN 2009  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-71  
DICTIONARY FILE UPDATES: 22 JUN 2009 HIGHEST RN 1159446-15-71

New CAS Information Use Policies: enter **HELP USAGE TERMS** for details.

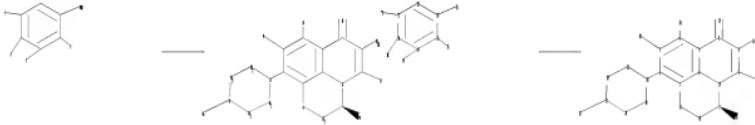
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stnqgen/stndoc/properties.html>

=>  
Uploading C:\Program Files\Stnexp\Queries\10578078cc.str



```
chain nodes :  
14 15 16 17 24 25 26 35 36 37 38 39  
ring nodes :
```

1 2 3 4 5 6 7 8 9 10 11 12 13 18 19 20 21 22 23 29 30 31 32  
 33 34  
 chain bonds :  
 2-18 3-24 4-26 7-14 8-15 9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36  
 ring bonds :  
 1-2 1-6 1-13 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 10-11 11-12 12-13  
 18-19 18-23 19-20 20-21 21-22 22-23 29-30 29-34 30-31 31-32 32-33 33-34  
 exact/norm bonds :  
 1-13 2-18 5-7 6-10 7-8 7-14 8-9 9-10 10-11 11-12 12-13 18-19 18-23  
 19-20 20-21 21-22 22-23  
 exact bonds :  
 3-24 4-26 8-15 9-25 11-16 17-21 29-39 30-38 31-37 33-35 34-36  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 29-30 29-34 30-31 31-32 32-33 33-34

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom  
 20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:CLASS 26:CLASS 29:CLASS  
 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:CLASS 36:CLASS 37:CLASS 38:CLASS  
 39:CLASS  
 fragments assigned product role:  
 containing 1  
 fragments assigned reactant/reagent role:  
 containing 29

## Stereo Bonds:

16-11 (Single Wedge).

## Stereo Chiral Centers:

11 (Parity=Don't Care)

## Stereo RSS Sets:

Type=Relative (Default). 1 Nodes= 11

L1 STRUCTURE UPLOADED

```
=> d 11
L1 HAS NO ANSWERS
L1 STR
```

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> file casreact	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	0.48	0.70

FILE 'CASREACT' ENTERED AT 10:11:11 ON 24 JUN 2009  
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT  
COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 21 Jun 2009 VOL 150 ISS 26

New CAS Information Use Policies, enter HELP USAGETERMS for details.

\*\*\*\*\*  
\*  
\* CASREACT now has more than 16.5 million reactions \*  
\*  
\*\*\*\*\*

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 11  
SAMPLE SEARCH INITIATED 10:11:16 FILE 'CASREACT'  
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS  
100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01  
  
FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0  
  
L2 0 SEA SSS SAM L1 ( 0 REACTIONS)  
  
=> s 11 sss full  
FULL SEARCH INITIATED 10:11:23 FILE 'CASREACT'  
SCREENING COMPLETE - 115 REACTIONS TO VERIFY FROM 10 DOCUMENTS  
100.0% DONE 115 VERIFIED 8 HIT RXNS 3 DOCS  
SEARCH TIME: 00.00.02  
  
L3 3 SEA SSS FUL L1 ( 8 REACTIONS)  
  
=> d ibib abs fhit tot

1.3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS on STN  
PRO B 94695-49-6  
SOL 68-12-2 DMF  
CON SUBSTAGE(1) room temperature -> 90 deg C  
SUBSTAGE(2) 6 - 8 hours

```

  RX(2)    ACT E 105-53-3

  STAGE(1)
  SOL 64-17-5 EtOH, 100-88-3 PdMe
  COM 20 minutes, zoom temperature
  STAGE(2)
  NOT 64-17-4 Mg
  CAT 64-17-3 CuCl2
  SOL 64-17-5 EtOH
  COM SUStAGE(1) zoom temperature
  SUStAGE(2) 30 minutes, zoom temperature
  SUStAGE(3) 3 1/2 hours, 90 deg C
  SUStAGE(4) 30 minutes, zoom temperature
  SUStAGE(5) 39 deg C > 55 deg C

```

```

STAGE [3]
ACT 3 34695-49-8
SOL 329-39-9 THF, 100-200-3 PhMe
CON SUBSTAGE [2] 30 - 35 deg C
SUBSTAGE [3] 35 deg C -> 5 deg C
SUBSTAGE [4] 2 hours, 0 - 5 deg C
SUBSTAGE [5] 5 deg C -> 25 deg C
SUBSTAGE [6] 5 deg C -> 25 deg C
SUBSTAGE [7] 30 minutes, 20 - 25 deg C

```

```

PRO T 94695-43-5
RKT F 94695-43-9
RKT M 124-135-4 7e0m
PRO L 124-135-4
RKT S 123-125-5 Mater
CON 3 hours, 80 - 30 deg C

RKT(4) RKT L 94695-30-8, O 122-31-0
PRO P 94695-30-6
RKT S 109-120-0
CON 0.987803(1) standard temperature > 120 deg C
CON 0.987803(1) standard temperature < 120 deg C

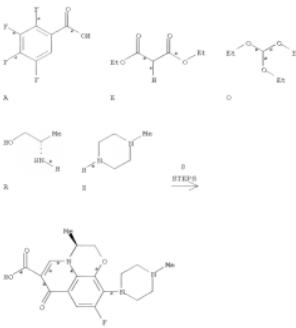
```

XX(5) ECT P 94714-58-6, R 2749-11-3  
 PRO S 110548-02-2  
 SOL 79-09-2, CDRCL2  
 CON 200000Z NOV 79 - 35 deg C  
 WURSTNOX(1) 35 deg C -> 5 deg C  
 WURSTNOX(2) 2 hours 0 - 5 deg C  
 WURSTNOX(4) 5 deg C -> 35 deg C  
 WURSTNOX(5) 2 hours, 30 - 35 deg C

300 (6)      KCT S 110545-02-2  
                KGT V 584-05-7 K2003  
                PRO U 106939-34-8  
                SOL 68-12-2 166

13 ANSWER 1 OF 3 CASREACT COPYRIGHT 2009 ACS ON STN (Continued)  
using aq. THF or an admixt. with other org. solvents to get highly pure  
levofloxacin hemihydrate having a single individual impurity which is  
<0.1% and is free from particulate matter and from the other enantiomer  
(R-form).

RK(36) OR 36 COMPOSED OF RK(1), RK(2), RK(3), RK(4), RK(5), RK(6), RK(7),  
 RK(8)  
 RK(36)  $\Delta + E + O + R + Z \longrightarrow AA$



RK(3) RCT A 3203-31-6  
RCT C 7719-09-7 SOC12

L7 ANSWER 3 OF 3 CIRCUITSTORY 2009 ACS on 87W (Continued)  
 CON SUBSTAGE(1) 120 deg C  
 SUBSTAGE(2) 3 hours, 120 deg C  
 SUBSTAGE(3) 50 minutes

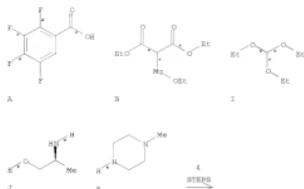
EX(7) RCT W 10598-93-0  
 RGT X 7647-00-0 SCL  
 PRO W 100986-99-8  
 SUBSTAGE(1) 10 hours, 80 - 120 deg C  
 CON SUBSTAGE(1) room temperature -> 80 deg C  
 SUBSTAGE(2) 6 hours, 75 - 80 deg C  
 SUBSTAGE(3) 1 hour, 70 - 75 deg C  
 SUBSTAGE(4) 1 hour, 75 - 20 deg C

EX(8) RCT W 100986-93-8 Z 129-01-3  
 RGT AA 110-06-1 Pyridine  
 PRO AA 100986-93-8  
 CON AA 110-06-1 Pyridine  
 CON 10 hours, room temperature -> 120 deg C  
 REFERENCES COUNT: 3 REFERENCES AND CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

Habte 06/24/2009

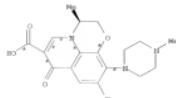
13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN  
ACCESSION NUMBER: 133157302 CASREACT  
TITLE: Studies on stereoselective synthesis of  
(S)-(-)-ofloxacin  
INVENTOR(S): Li, Xian-Ming, Geng, Shang, Xing, Zhou, Sixiang  
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Anhui College  
of Traditional Chinese Medicines, Hefei, 230039,  
People's Republic of China  
SOURCE: Shengguo Yunnan Huamei Xizhi (2000), 10(4), 276-278  
COUNTRY: CHINAFI: 1200-1025-0108  
PUBLISHER: Shengguo Yunnan Huamei Xizhi, Xianjin  
DOCUMENT TYPE: JOURNAL  
LANGUAGE: Chinese  
ABSTRACT: (S)-(-)-Ofloxacin was synthesized from 2,3,4,5-tetrafluorobenzoic acid by chlorination, condensation with di-Et malonate, partial hydrolysis, cyclization, and substitution with (S)-(+)-3-methoxypropanol, cyclization, hydrolysis, and substitution with N-methylpiperazine. The overall yield from 2,3,4,5-tetrafluorobenzoic acid and was 39.4%.

EX(10) OF 10 COMPOUNDS OF EX(1), EX(2), EX(3), EX(4)  
EX(12) A + B + I + J + X ==> S



13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
EX(4) R 109-01-3, O 100986-89-8  
TSD 2 100986-91-4  
SOL 67-009-3 DMDO

13 ANSWER 2 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)



S YIELD 82%

EX(11) RCT A 1201-31-6

STAGE(1)  
RCT R 109-01-3 R0C12  
SOL 68-12-2 DMF

STAGE(2)  
RCT R 207746-86-9  
SOL 108-88-3 THF

STAGE(3)  
RCT R 104-15-4 TeOH  
SOL 7152-18-5 Water

PRO C 94095-50-0

EX(2) RCT I 122-51-0, C 94095-50-0

STAGE(1)  
SOL 108-24-7 Ac2O

STAGE(2)  
RCT J 2743-11-3  
SOL 68-00-2 CR2C12

STAGE(3)  
RCT L 544-99-7 KC003  
SOL 68-12-2 DMF

PRO K 100939-34-8

EX(3) RCT K 100939-34-8

RCT P 7647-01-0 HC1

PRO O 100986-89-8

SOL 68-19-7 AcOH

13 ANSWER 3 OF 3 CASREACT COPYRIGHT 2009 ACS on STN (Continued)  
ACCESSION NUMBER: 13015530 CASREACT

TITLE: Preparation of racemic and optically active ofloxacin and related derivatives

INVENTOR(S): Mitischer, Lester A.; Chu, Daniel T.; Patisonti, Somsak; Patisonti, Oma

PATENT ASSIGNEE(S): U.S.A., 7 pp

SOURCE: C00XAN

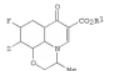
DOCUMENT TYPE: P

LANGUAGE: English

DATE: 1994-05-11, 1994-05-11

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4777223	A	19880111	US 1984-55832	19800425
US 4800254	A	19890502	US 1984-55833	19800425
PRIORITY APPLN. INFO.: I			US 1984-55832	19800425
OTHER SOURCE(S):			MAPAT 110+75530	

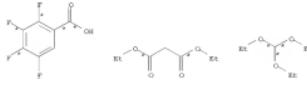


I

AS The title compds. I (R1 = H, Cl-4 alkyl, PhCH3; Z = 4235H) 24, 25 = H, alkyl, alkanoyl, alkanoyleamido, substituted amino; R4R5H = (un)substituted aliphatic (1-4C) and heterocyclic (1-4C) (wherein the racemate of ofloxacin exhibits antibacterial properties) were prepared. (-)-I (R1 = Et; Z = F) (prepared by the method of Example 1) was dissolved in THF and NaH solution, and after working up, the solid obtained was dissolved in THF and NaH solution to give (-)-I (R1 = H; Z = F) (prepared by the method of Example 1).

EX(8) OF 102 COMPOUNDS OF EX(4), EX(3), EX(5), EX(6), EX(13), EX(9)

EX(8) H + Y + I + K + B ==> N

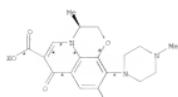
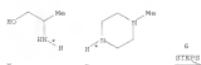


N

Y

I

K



37

306149 3072 H 1203-31-6

304 (3) 3072 E 94695-48-4, F 105-53-3  
39.0 G 94695-50-8

36151 362 94695-50-0, 1 322-53-0

206 162 2004 52 94724-58-6A 25 2749-33-3

300 L 110548-02-2

SOL 129-99-9 78F

307 Q 7732-18-5 Materx

SOL 7732-18-5 Water

RECORD. 3  
FORMAT